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HEADS UP!

## Materials Capability Review draws near

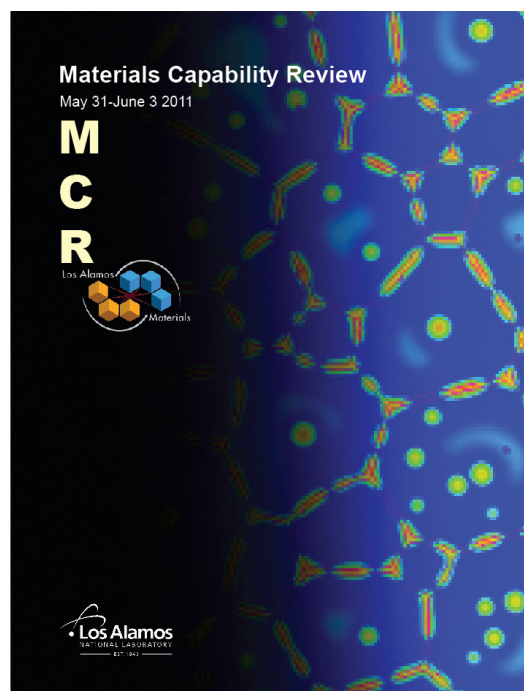
Materials research performed by Laboratory scientists will be the focus of the 2011 Materials Capability Review, to be held May 31-June 3.

In poster and presentation sessions, the review will highlight recent materials research in radiation environments, for clean energy, for nuclear energy—with a focus on actinides studies, and experiments performed at the Los Alamos Neutron Science Center (LANSCE). More than 20 groups from 8 divisions will participate in the review, which supports the Laboratory's goal of being a capabilities-based national security science laboratory.

A distinguished nine-member review committee from universities and national laboratories and chaired by Gary Was of the University of Michigan will evaluate the quality of science within the materials capability.

Members of the Laboratory's materials community are invited to attend. Organized by the Experimental Physical Sciences Directorate, the review will be held at the Oppenheimer Study Center and wrap up Friday at LANSCE.

For the agenda, please see [int.lanl.gov/orgs/adepts/docs/MCR\\_agenda\\_5-19-2011.pdf](http://int.lanl.gov/orgs/adepts/docs/MCR_agenda_5-19-2011.pdf).



The cover story this month touts the Materials Capability Review. This is a big deal that we go through each year. Almost a week long, and the preparatory phase begins months in advance. Why do we bother? It has several purposes:

1) Simply put, it is a requirement of our operating contract. As a capabilities-based Laboratory, the NNSA requires review of our science & technology in order to gauge the effectiveness of our management structure in nurturing world-class S&T. The good news is that the output is not a simple grade. Which brings us to #2.

2) The review committee becomes our advocates. Of course, we must show them that we have outstanding science and that we make a difference to Laboratory missions. But we also show them some warts. And then they help us to think through how to address those issues, and they put in a helpful word for us with PADSTE and the Director's office. For example, the review committee was instrumental in helping us to convince the powers-that-be of our need for upgrades to our electron microscopy instrumentation a few years back. And, this year, they want to know if we are making progress on a plan for sustainable funding to maintain and operate those scopes (answer: we're getting there, but it's slow going).

3) We get to strut our stuff to Los Alamos upper management. It is a really good thing for our AD and our PAD on up to become more closely acquainted with the great work we do. The timing is perfect, because our new director should be announced right about the time of the review. We'll have this gorgeous briefing book all ready for him or her, along with some (hopefully!) strong words of praise from the committee for us.



**'Given our responsibility for stewardship of the Materials Capability, it is an important part of my job to spend some quality time thinking about the breadth and depth of materials work going on across the Lab and opportunities for the future. Putting together this review gives me the opportunity to do just that.'**

4) Despite how it interrupts our "real" work, the preparatory phase is useful in fostering dialogue across the various organizations and management across the Lab that do materials work. As the lead POC this year, working closely with Toni Taylor, we formed a team of colleagues to organize the review. Besides MST and MPA, we had strong involvement from LANSCE and T, along with support from P, C, WX, N and more. Given our responsibility for stewardship of the Materials Capability, it is an important part of my job to spend some quality time thinking about the breadth and depth of materials work going on across the Lab and opportunities for the future. Putting together this review gives me the opportunity to do just that.

So, for those of you who have had to devote some of your valuable time to helping us with the review, thank you very much and know that it is critically important to our future well-being to take these reviews seriously. From within MST, I want to especially thank Dave Teter, Chris Stanek, Andy Nelson, and Yong Wang, each of whom will be making a presentation to the committee. I recognize, as well, numerous poster presenters and early-career dialogue participants who are contributing substantially to the overall impression that we make on the review committee.

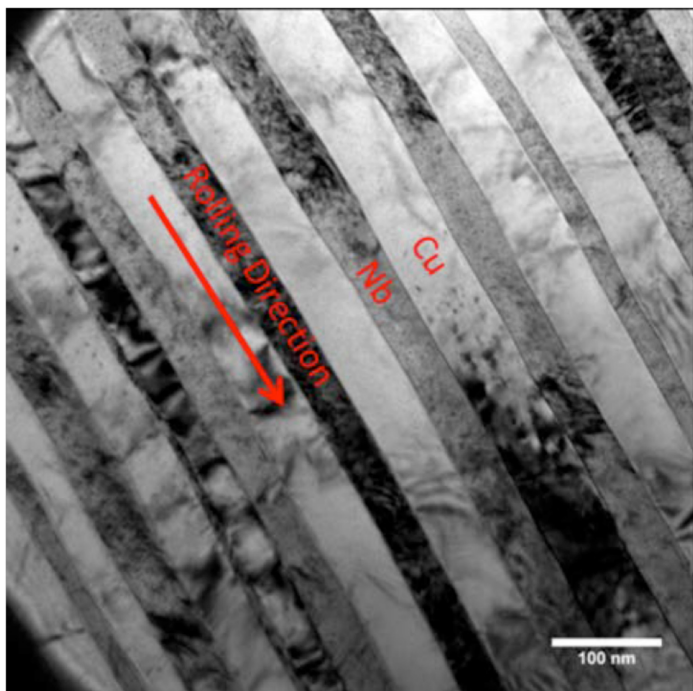
For those of you who haven't yet gotten involved, consider joining us at one or more of the open sessions. We have posted the agenda on our internal Web site at [http://int.lanl.gov/orgs/adepts/docs/MCR\\_agenda\\_5-19-2011.pdf](http://int.lanl.gov/orgs/adepts/docs/MCR_agenda_5-19-2011.pdf). Or just ask your group office or the division office for a copy of the agenda. I hope to see you there!

*MST Division Leader Wendy Cieslak*

## Bulk nanolamellar multilayer composites fabricated via severe plastic deformation

Compared with micron-sized polycrystalline aggregates, nanolamellar metallic composites have a variety of useful, extraordinary properties including high strength, imperviousness to irradiation, and excellent shock resistance. These properties are a result of both the interface structure, which serve as a recombination site for defects, and the density of heterophase interfaces. Los Alamos scientists have used physical vapor deposition (PVD) as an effective method for controlled synthesis of interface structures with nominal layer thicknesses as low as 2.5 nm. This type of deposition process is known as “bottom up” synthesis.

LANL researchers have employed accumulative roll bonding (ARB) as an alternate “top-down” technique to fabricate nanolamellar metallic composites. Beginning with two 1-mm thick sheets of high-purity polycrystalline copper and niobium, scientists performed repeated stacking and roll bonding in a rolling mill to fabricate multilayers with nominal layer thickness of approximately 10 nanometers (similar to PVD). The overall sample thickness of 140 microns was much thicker than nanolamellar metallic composites formed from the PVD process. The team used texture information gathered from neutron diffraction and transmission electron microscopy at various layer thicknesses formed along the synthesis pathway to investigate interface structure. A characteristic texture, distinct from both the standard rolling textures and the



A bright field transmission electron microscopy view of a copper (Cu)/niobium (Nb) nanolamellar metallic composite formed by the ARB method. The nominal layer thickness was 48 nanometers.

PVD texture, saturated at a layer thickness of 50 nm and remained stable at lower layer thicknesses. These results indicated that rolling and ARB could be used to fabricate nanolamellar metallic composites with consistent interface structure and a high density of heterophase interfaces. The team will test the stability of these interfaces and their ability to mitigate damage under other extreme conditions such as irradiation and shock deformation.

Laboratory Directed Research and Development (LDRD) and the DOE Basic Energy Sciences – Energy Frontier Research Center for Materials at Irradiation and Mechanical Extremes (CMIME) funded different aspects of the research. John Carpenter, Nate Mara, Rob Dickerson, Rod McCabe, Tom Wynn, and Duncan Hammon (Metallurgy, MST-6), Sven Vogel (Lujan Neutron Scattering Center, LANSCE-LC), and Irene Beyerlein (Fluid Dynamics and Solid Mechanics, T-3) performed the work. The research supports the Laboratory’s Energy Security mission area and the Materials for the Future capability.

## Comparing quasi-static and dynamic deformation behavior in lightweight armor alloys

To meet the demand for stronger and lighter armor material, the deformation mechanisms of these alloys must be understood. Therefore, Los Alamos researchers measured the mechanical response of aluminum alloys 5083, 5059, and 7039 for compression and shear in both the quasi-static (0.001 s<sup>-1</sup>) and dynamic (approximately 2000 s<sup>-1</sup>) strain rate regimes. Orientation image mapping enabled detailed analysis of the specimens post-mortem with larger emphasis on the top-hat shear samples. The orientation image map reveals information about how the microstructure deformed in a shear manner. The quasi-static and dynamic strain rates caused dramatically different deformation behavior in shear.

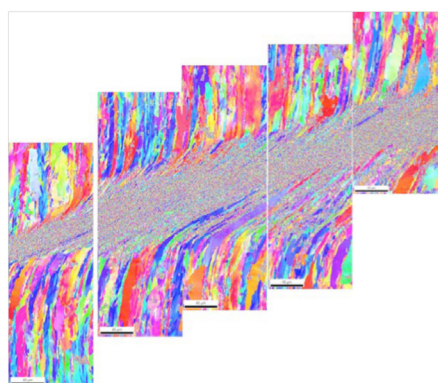
The specimens tested at quasi-static rates exhibited hardening as displacement was increased. At the slower strain rates, all of the alloys had a relatively large volume of highly deformed material, with 5083 and 5059 having the largest affected volume. Specimens from the dynamic strain rates all formed highly compact shear bands across the sheared area, with 7039 having the tightest shear band (see figure). These shear bands along with an absence of hardening during deformation indicate a catastrophic damage event at the higher strain rates. Higher resolution orientation image mapping has shown that between the three alloys there are varying degrees of order within the shear bands.

*continued on page 4*

**Dynamic...** The researchers conclude that these alloys are all suitable for armor. Both the 5083 and 7039 are already in use. The 5059 alloy has better mechanical response than the 5083 alloy, and with its improved corrosion resistance over 7039, would appear to be a suitable replacement for 5083 and 7039 if the application would be exposed to a corrosive environment. Researchers include Sara Pérez-Bergquist, Ellen Cerreta, Rusty Gray, Carl Trujillo and Mike Lopez (Structure/Property Relations, MST-8).

The DoD/DOE Joint Munitions Program (Rusty Gray, LANL Program Manager) funded the work, which supports the Lab's Global Security and Nuclear Deterrence mission areas and the Materials for the Future capability.

*Technical contact: Sara Pérez-Bergquist*

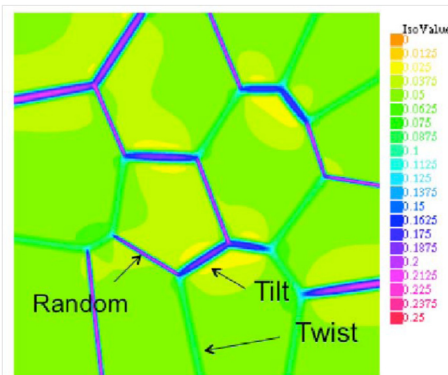


*Orientation image map of the shear zone of an aluminum alloy 7039 top hat after dynamic deformation.*

## Atomistic and mesoscale simulations of diffusion in $\text{UO}_{2\pm x}$ nuclear fuels

Species transport in uranium oxide ( $\text{UO}_{2\pm x}$ ) nuclear fuels influences fuel performance during reactor operation and has implications for accident scenarios. For example, fission gas bubbles cause swelling, mechanical interaction with the cladding, and decreased thermal conductivity of the fuel. Fission gas released to the plenum increases the pressure on the clad walls. Los Alamos scientists and university collaborators have studied diffusion of oxygen, uranium, and fission gases in nuclear fuels using simulation techniques ranging from density functional theory, molecular statics, and kinetic Monte Carlo at the atomic length scale to diffusion theory and phase field simulations describing microstructure evolution at the mesoscale. The simulations highlight the impact of the  $\text{UO}_{2\pm x}$  oxygen content on species transport and reveal competition between different grain boundary types for segregation of fission gases.

Both diffusion of fission gases and thermal conductivity depend on the  $\text{UO}_{2\pm x}$  oxygen content. Therefore, scientists must understand oxidation in order to predict fuel performance. Density functional theory directly calculates the diffusion coefficient for fission gas and



*Simulation of xenon concentration after 55 hours in an idealized microstructure with a homogeneous initial xenon fraction of 0.05. The microstructure contains three different types of grain boundaries (random,  $\Sigma 5$  tilt and  $\Sigma 5$  twist), and the domain size is 100 nanometers.*

uranium transport. For oxygen diffusion, an additional kinetic Monte Carlo model captures the influence of oxygen aggregation for  $\text{UO}_{2\pm x}$  with higher oxygen content. Atomistic simulations based on empirical potentials quantify the interaction of the diffusing species with the fuel microstructure, both grain boundaries and dislocations. The findings are collected in diffusion and phase field models that are solved using finite element methods.

David Andersson, Blas Uberuaga, Luis Casillas, Pankaj Nerikar, and Chris Stanek (Structure/Property Relations, MST-8); Cetin Unal (Computer, Computational, and Statistical Sciences, CCS-DO); R.K. Behera, C. Deo, and T. Watanabe (Georgia Institute of Technology) performed the research.

The DOE Nuclear Energy Advanced Modeling and Simulation program and the LDRD program funded different aspects of the work, which supports the Lab's Energy Security mission area and the Materials of the Future and the Information Science and Technology capabilities.

*Technical contact: David Andersson*

## Celebrating service

Congratulations to the following MST Division employee celebrating a service anniversary this month:

Angelique Neuman, MST-16

15 years

## MST NEWS

Published monthly by the Experimental Physical Sciences Directorate. To submit news items or for more information, contact Karen Kippen, EPS Communications, at 606-1822, or [kippen@lanl.gov](mailto:kippen@lanl.gov).



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## Annual LANL Recycle and Reuse Event to be held June 16

What a great opportunity to complete your office or work space spring cleaning AND contribute to an important recycling event here at the Lab!



Are your supply cabinets stuffed with unwanted but useable items? Things you ordered by mistake or in the wrong quantity? Do you have cartridges for printers that you no longer use? This is the event for you! You can donate these unwanted supplies to the Recycle and Reuse Event so that others at the Lab can benefit.

Need to set up new offices for your students and postdocs? This would be the place to visit to gather the office supplies and perhaps even some furniture that you need. Or maybe just browse around for some office items you need but never got around to placing that order. It's all free for the taking!

LANL's "Recycle and Reuse Event" will be held on Thursday June 16 between 9 a.m. and 2 p.m. at the Canyon School complex and is open to all badged employees. Office supply vendors will also be present. Give-aways and many special door prizes will be awarded to lucky visitors.

Please be sure to gather up all your unwanted/unneeded office supplies and (working) equipment between now and the collection dates of June 14 and 15. Clean out that storage closet and desk for all those supplies you ordered so long ago but never used! The event's inventory depends on you; recycle a little—reuse a little. Your EMS POC will be glad to assist you; a list of possible collection items will soon be sent to you electronically and also posted at your group office. Any questions or need further information? Contact your EMS POC (Physics: Steve Glick; MPA: Cathy Padro; MST: Jim Coy; LANSCE: Frances Aull).

If you'd like to help further, items and office supplies can be dropped off on June 14 and 15 between 9 a.m.– 4 p.m. at Canyon School rooms 164, 169, 172. If you can't drop off your items, let your EMS POC know and he or she will make other arrangements. Also, if you don't have space for storing larger items (chairs, furniture) until June, the Salvage Operations Team has agreed to collect and hold items for the event. Send a request for a salvage pickup and mark items "LANL R&R Event."

With your help we can make the Laboratory clean and green!

## HeadsUP!

### Your chance to slip safely!

The Voluntary Protection Program (VPP) Office has researched the use of a slip simulator used by United Parcel Service (UPS) and designed by Virginia Tech that has significantly reduced slip injuries at UPS. As a result the Lab has purchased three simulators and is taking a similar approach to address slip injuries.

The objective of a slip simulator is to provide a kinetic learning module ("learn by doing") that has participants experience a slippery surface without the risk of falling due to a built-in fall arrest system. According to VPP Project Leader Bethany Rich, "This experience raises awareness of the importance of walking speed, selection of shoe soles, and placement of your center of gravity."

*A LANL slip simulator reproduces conditions that lead to slip and fall accidents, in this case carrying a box across a very slick surface. Trainees on the system are also tasked with walking—and not slipping—while texting on a Blackberry. A combination of modified footwear, a safety harness and a highly polished floor surface create the perfectly controlled accident waiting to happen.*



### Joint efforts behind unique safety initiative

"While many improvements have been made by Worker Safety and Security Teams (WSSTs) and managers to improve our facilities and walking surfaces across the Lab, we will never have a perfect environment," said Rich, "and as Human Performance Improvement (HPI) reminds us, being humans, we will always make mistakes. This [initiative] offers workers one more tool to help take better care of ourselves and each other."

"We're pleased that the number of slips, trips and falls is starting to decline, but we would like to see the number of injuries reduced even further," said Chris Cantwell, associate director for Environment, Safety, Health and Quality. "The combination of VPP efforts, WSST participation, HPI initiatives, and Behavior Based Safety activities have resulted in this unique and forward-thinking safety initiative that I believe will take us to a new level of safety performance."

When the slip simulators are ready for general use, the VPP Office will notify workers how to sign up for free workshops.